Valence offsets of ternary alloy heterojunctions $In_xGa_{1-x}As/In_xAl_{1-x}As$*

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The ternary alloy heterojunctions $In_xGa_{1-x}As/In_xAl_{1-x}As$ are important materials which have been widely used in microwave and photoelectric devices[1]. The alloy heterojunctions $In_xGa_{1-x}As/In_xAl_{1-x}As$ ($x=0.3$) have great potential use in high electron mobility transistors (HEMTs), heterostructure insulated-gate FFTs (HIGFETs) and resonant tunneling diodes (RTDs). When x rises to 0.53, $In_xGa_{1-x}As/In_xAl_{1-x}As$ can be widely used in the high-speed electronic devices[2]. The valence-band offset (the value of ΔE_v) at semiconductor heterointerface is a key parameter for electronic properties of heterojunction and superlattice, which has great significance in theoretical calculation and experimental research.

Although there have been many theoretical researches about valence-band offsets (VBO's, i.e. ΔE_v) at lattice-matched and lattice-dismatched heterojunctions constructed by elements or compound semiconductors in recent years[3], the theoretical studies on $\Delta E_v(x)$ at alloy heterojunctions are still very scarce. In this note, we study $\Delta E_v(x)$ at the alloy heterojunctions $In_xGa_{1-x}As/In_xAl_{1-x}As$ by the use of LMTO-ASA band method and the average-bond-energy method[4] in conjunction with the cluster expansion method for the first time. The results of our calculation are in very good agreement with available experimental data, showing that the average-bond-energy method in conjunction with the cluster expansion method well fits the calculation of $\Delta E_v(x)$ at alloy-type heterojunctions.

1 Average bond energy E_m of five-ordered alloy structures of $In_lGa_{4-l}As_4$ and $In_lAl_{4-l}As_4$

In this note, the band structures of three-component alloy $In_lGa_{4-l}As_4$ and $In_lAl_{4-l}As_4$ are calculated with LMTO-ASA method. Among the five ordered structures ($l=0$, 1, 2, 3, 4), $l=0$ and 4 are the zinc-blende (ZB) structure; $l=2$ the CuAu structure (labeled by $L1_0$)

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and $l=1$ and 3 are Luzonite ($L1_2$) structures[5]. The lattice constants of five ordered structures can be obtained as the average of the bulk-materials GaAs, AlAs and InAs in proportion to their contents. After getting the self-consistent band structures for the five ordered structures, we determine their bonding energy, antibonding energy, and average bond energy by

$$E_b=\frac{1}{MN}\sum_{n=1}^{M}\sum_{\mathbf{k}}E_n(\mathbf{k}), \tag{1}$$

$$E_a=\frac{1}{MN}\sum_{n=M+1}^{2M}\sum_{\mathbf{k}}E_n(\mathbf{k}), \tag{2}$$

$$E_m=(E_b+E_a)/2, \tag{3}$$

respectively, where N is the number of unit cells and M the number of valence bands. For the ZB, $L1_0$ and $L1_2$ structures, M is evaluated by 4, 8 and 16, respectively. The special-K-point method[6] is adopted for the summation over the Brillouin zone. Two special K points are used for ZB and $L1_0$ structures and only one special K point is used for the $L1_2$ structure.

2 Parameter of band offsets ($E_m(x)-E_v(x)$) of the three-component alloy

The value of the band offsets of heterojunction is mainly determined by the parameter of band offsets (E_m-E_v) of the five ordered semiconductor structures. We can obtain the average bond energy $E_m(x)$ and the valence-band maximum $E_v(x)$ for $In_xGa_{1-x}As$ and $In_xAl_{1-x}As$ by making use of the cluster expansion method, in terms of the data of the five ordered structures listed in table 1, i.e.

$$E_m(x)=\sum_l P_l(x)E_m^l, \tag{4}$$

$$E_v(x)=\sum_l P_l(x)E_v^l, \tag{5}$$

where the statistic weight is

$$P_l(x)=\binom{4}{l}x^l(1-x)^{4-l}. \tag{6}$$

Table 1 Results of the parameter of band offsets ($E_m(x)-E_v(x)$) for the five ordered structures and alloys respectively (all in eV)

	$In_lGa_{4-l}As_4$		$In_lAl_{4-l}As_4$	
	E_m-E_v	$E_m(x)-E_v(x)$	E_m-E_v	$E_m(x)-E_v(x)$
$l=0$	−0.015	−0.016	0.524	0.515
$l=1$	0.005	0.008	0.401	0.400
$l=2$	0.034	0.037	0.279	0.294
$l=3$	0.071	0.071	0.198	0.197
$l=4$	0.108	0.109	0.108	0.109

The regressed two-order polynomials for the parameter of band offsets $(E_m(x)-E_v(x))$ is for $In_xGa_{1-x}As$,

$$E_m(x)-E_v(x)=0.036x^2+0.089x-0.016; \tag{7}$$

for $In_xAl_{1-x}As$,

$$E_m(x)-E_v(x)=0.073x^2-0.479x+0.515. \tag{8}$$

The calculated results are also listed in table 1.

3 Determination of $\Delta E_v(x)$ at ternary alloy-type $In_xGa_{1-x}As/In_xAl_{1-x}As$ heterojunction

After obtaining the band offset parameter from eqs. (7) and (8), $\Delta E_v(x)$ can be determined according to the formula:

$$\Delta E_v(x)=[E_m^B(x)-E_v^B(x)]-[E_m^A(x)-E_v^A(x)], \tag{9}$$

which can be shown as the regressed two-order polynomials:

$$\Delta E_v(x)=0.037x^2-0.567x+0.531. \tag{10}$$

In the above expression, it can be seen that the $\Delta E_v(x)$ value of $In_xGa_{1-x}As/In_xAl_{1-x}As$ is a function of x, and it decreases with the increase of x, i.e. with the increase of the In content (i.e. the decrease of the Ga and Al content). Eq. (10) shows that the two-order coefficient which is a characterization of the bending of $\Delta E_v(x)$ curve is very small (0.037), the value of $\Delta E_v(x)$ changing with x is nearly linear. Therefore, the $\Delta E_v(x)$ values of the alloy-type $In_xGa_{1-x}As/In_xAl_{1-x}As$ heterojunctions can be obtained approximately by linear regressing from the ΔE_v values of the bulk materials GaAs, AlAs and InAs.

4 Comparison between theoretical and experimental results

Comparing the $\Delta E_v(x)$ values of $In_xGa_{1-x}As/In_xAl_{1-x}As$ (listed in table 2, where $x=y$ and x is very close to y) with the experimental data, we found that they agree with each other for a different composition x, which indicates that the average-bond-energy method in

Table 2 Experimental data of valence-band offsets ΔE_v of three-component alloy-type $In_xGa_{1-x}As/In_yAl_{1-y}As$ heterojunctions compared with the theoretical data in this work (all in eV)

	This work	Ref. [1]	Ref. [1]	Ref. [2]	Ref. [7]	Ref. [8]	Ref. [9]
$Q_c(=\Delta E_c/\Delta E_g)$	0.656[a)]	0.66	0.62	0.68		0.72	0.650
$\Delta E_v(x, y)$							
(0, 0)	0.531				0.55		
(0.3, 0.29)	0.368	0.36	0.41				
(0.3, 0.3)	0.364						
(0.52, 0.52)	0.246					0.22	
(0.53, 0.52)	0.244			0.22			

a) When $(x, y)=(0.3, 0.29)$, $\Delta E_g=1.07$, $\Delta E_c=\Delta E_g-\Delta E_v=0.702$, $Q_c=\Delta E_c/\Delta E_g=0.656$.

conjunction with the cluster expansion method is effective for calculating the valence-band offsets of multi-component alloy-type heterojunctions.

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